

image, as we have seen in orthorhombic $Ti_2Nb_{10}O_{29}$. The unit-cell dimensions (which are listed in Table 8) together with the ideal and the probable distorted atomic arrangements for each can readily be predicted, and it is therefore a simple problem to compute theoretical Guinier diffraction patterns to compare with those made from laboratory preparations. Such an aid is considered indispensable in a problem of this kind.

Attempts were made to prepare the two intermediates $n=2$ and 5. The low temperature forms of Nb_2O_5 and Ti_2O_5 were weighed and heated together at small temperature intervals from 700 °C. through to the quenched liquidus. $Ti_4Nb_2O_{13}$ (i.e. $n=2$) was not found in any of these, and all specimens consisted of $TiNb_2O_7$ plus rutile. $TiNb_{14}O_{37}$ ($n=5$) gave a bewildering variety of diffraction patterns bearing considerable similarities to one another as well as to αNb_2O_5 , the high temperature form, but containing diffuse regions and many additional lines. At no time could it be stated that the Guinier patterns consisted solely of one or other of the two predicted forms, and evidently considerable crystalline disorder was present as well.

In some respects the cell dimensions reported for Nb_2O_5 in certain of its forms resemble those for $Me_{18}O_{45}$ in Table 8, the high-temperature form to the

monoclinic and the γ form to the orthorhombic.* Similarities between the γ form and an Me_3O_8 oxide (U_3O_8) have also been noted (Holser, 1956). Disorder as well as distortion undoubtedly plays an important role in these structures, and additional reference to this will be made elsewhere.

It appears, therefore, that $TiNb_2O_7$ and $Ti_2Nb_{10}O_{29}$ are the only representatives of the series $Me_{3n}O_{8n-3}$ which can be identified with certainty within $TiO_2-Nb_2O_5$. Other members may eventually be found in chemical systems of a related kind.

References

- ANDERSSON, S., COLLÉN, B., KUYLENSTIerna, U. & MAGNÉLI, A. (1957). *Acta Chem. Scand.* **11**, 1641.
 HÄGG, C. & MAGNÉLI, A. (1954). *Revs. Pure Appl. Chem. Australia*, **4**, 235.
 HOLSER, W. T. (1956). *Acta Cryst.* **9**, 196.
 ROTH, R. S. & COUGHANOUR, L. W. (1955). *J. Res. Nat. Bur. Stand. Wash.* **55**, 209.
 WADSLEY, A. D. (1958). *J. Proc. Roy. Soc. N.S.W.* **92**, 25.
 WADSLEY, A. D. (1961). *Acta Cryst.* **14**, 660.
 ZVINCHUK, R. A. (1959). *Soviet Physics, Crystallography*, **3**, 750.

* The nomenclature is that of Zvinchuk (1959) who has tabulated the unit-cell dimensions of several polymorphs of Nb_2O_5 . His setting for αNb_2O_5 is in striking agreement with 'monoclinic $TiNb_{14}O_{37}$ '.

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Piezo-Optic Birefringence in NaCl Structure Crystals. Part I. Theory

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Following Bragg's method, expressions for continuum, dipole and Coulomb anisotropies as well as ionic polarizability and density changes are given for the piezo-optic birefringence in crystals. Certain simplified assumptions lead to the evaluation of the strain-optical coefficients P_{11} and P_{12} from the observed difference ($P_{11}-P_{12}$). Expressions for Mueller's strain polarizability constants are seen to depend on wavelength and temperature.

1. Introduction

Attempts have been made by Banerjee (1927), Herzfeld (1928), Herzfeld & Lee (1933) and Mueller (1935a) to explain the photoelastic effect in cubic crystals. Banerjee developed a theory on the lines suggested by Bragg (1924a, b), Herzfeld & Lee adopted the lattice sum method of Madelung, and Mueller based his calculations on Born's theory of crystal lattices. While all these investigators considered the anisotropies arising from the Lorentz-Lorentz and Coulomb forces, Mueller considered the additional effect of strain on ionic polarizabilities. Mueller's

treatment shows that Bragg's & Born's methods are equivalent. All these attempts, however, have had a limited success. Discussions (Poindexter, 1955) based on quantum-mechanical considerations also do not lead to a satisfactory solution of the problem.

Mueller has drawn attention to the serious errors found in Banerjee's work. Banerjee's approach though essentially sound, does not take into account all possible factors that contribute to the observed birefringence. Mueller's work, in spite of its distinctive advance over the work of Banerjee and of others, nevertheless itself suffers from certain serious draw-

backs. For example, his expressions for the birefringence involve assumptions which recent experiments have shown to be untenable. These and other aspects have been considered in the following treatment which is based on Bragg's method. The theory outlined here yields quantitative results in agreement with experimental facts. The results have been discussed in Part II of the work.

2. Phenomenological theory

The phenomenological theory of photo-elasticity was given by Pockels in 1889. According to this theory the number of strain-optical constants that would be necessary to describe the photoelastic properties of a crystal depends on the class to which the crystal belongs. In the case of cubic crystals of the T_d , O and O_h classes only three optical constants P_{11} , P_{12} and P_{44} are necessary completely to define the photo-elastic effect.

Suppose that a rectangular bar of a cubic crystal with edges parallel to [100], [010], [001] is stressed along the Z -axis [001]. The refractive index of this stressed bar will be different for light vibrations parallel and perpendicular to the direction of stress. Let the indices be denoted by n_z and n_x and let the propagation of light be in the y -direction. The following expressions then define the strain-optical coefficients P_{11} and P_{12}

$$\begin{aligned} dn_x &= n_x - n = -P_{12}(n^3/2)\varepsilon, \\ dn_z &= n_z - n = -P_{11}(n^3/2)\varepsilon, \end{aligned} \quad (1)$$

where n is the refractive index of the unstressed crystal and ε the strain induced in the Z -direction due to the application of a stress.

A similar bar of the crystal with orientations [101], $[10\bar{1}]$, [010] when stressed along the Z -direction [101] or $[10\bar{1}]$ and the light is observed along [010], will yield the strain-optical coefficient P_{44} given by the expression

$$n'_z - n'_x = -P_{44}(n^3/2)\varepsilon', \quad (2)$$

where n'_z and n'_x are the refractive indices and ε' is the corresponding strain.

The treatment in Parts I and II will be confined to a discussion of the coefficients P_{11} and P_{12} .

3. Change in refractive index due to anisotropic fields

Following Burstein & Smith (1949) we will assume that the Lorentz-Lorenz equation is the proper form for representing the refractive index of cubic crystals. The unequal changes in the refractive index resulting from deformation may be considered to arise from the following anisotropies:

1. The Lorentz-Lorenz anisotropy due to the material continuum.
2. The Lorentz-Lorenz anisotropy due to the

dipoles within a cavity of lattice dimensions. This we shall call the dipole anisotropy.

3. Coulomb anisotropy due to the presence of positive as well as negative ions within the cavity.

The Lorentz-Lorenz anisotropy has been calculated by Mueller (1935*b*) on lines suggested by Havelock (1908). He has shown that for a medium strained in the Z -direction, where the strain ellipsoid has the axial ratio $1:1:1+\varepsilon$, the refractive index n_x for light vibration in the X -direction is given by (Brayborn, 1953)

$$3(n_x^2 - 1) = 4\pi N\alpha\{(n_x^2 + 2) + K_x(n^2 - 1)\} \quad (3)$$

with similar expressions for vibrations in the Y and Z directions. Here $K_x = K_y = 2\varepsilon/5$, $K_z = -4\varepsilon/5$, α is the polarizability of the molecule and N is the number of such molecules in unit volume of the substance. Equation (3) applies only to isotropic bodies.

In ionic crystals of the NaCl type besides the anisotropy of the continuum, two additional anisotropies, namely the dipole and Coulomb anisotropies, are present during deformation. These will further alter the refractive indices, n_x etc. of equation (3). In order to evaluate them, following the treatment of previous workers, we assume a cavity spherical in shape and of radius greater than $\sqrt{3}r$ and less than $2r$, where $2r$ is the lattice constant. When this cavity is subjected to a uniaxial stress, in the direction of one of the edges of the cell, the sphere changes over to an ellipsoid and the ions originally arranged in a cubic lattice will be re-arranged in a rectangular lattice of dimensions $2x, 2y, 2z$, when the centre of the cell is chosen as the origin of the co-ordinate system.

Let the polarizabilities of the ions be α_j in the unstressed condition and let a beam of light travel through the cavity with its electric vector of amplitude E_{tz} in the Z -direction. The induced dipole moment of the ions will be

$$(\mu)_{jz} = \alpha_j E_{\text{eff}}, \quad (4)$$

where E_{eff} is the effective electric field in the cavity, when the interaction of the ions is neglected, $(\mu)_{jz}$ represents the dipole moment of the negative or the positive ion according as j is 1 or 2. If the interaction is taken into account, we proceed as follows:

A doublet at the point (x, y, z) whose moment components are μ_x, μ_y and μ_z will give rise to a field at the origin. In Heaviside units which we shall use throughout this paper x, y and z components of this field will be

$$\begin{aligned} E_{x0} &= \frac{\mu_x}{4\pi} \frac{3x^2 - R^2}{R^5} + \frac{\mu_y}{4\pi} \frac{3xy}{R^5} + \frac{\mu_z}{4\pi} \frac{3xz}{R^5} \\ E_{y0} &= \frac{\mu_y}{4\pi} \frac{3y^2 - R^2}{R^5} + \frac{\mu_z}{4\pi} \frac{3yz}{R^5} + \frac{\mu_x}{4\pi} \frac{3xy}{R^5} \\ E_{z0} &= \frac{\mu_z}{4\pi} \frac{3z^2 - R^2}{R^5} + \frac{\mu_x}{4\pi} \frac{3xz}{R^5} + \frac{\mu_y}{4\pi} \frac{3yz}{R^5}. \end{aligned} \quad (5)$$

Here $R^2 = x^2 + y^2 + z^2$.

There will thus be at the centre a resultant field due to all the dipoles contained in the cavity. If the incident field is polarized in the Z -direction and the centre is occupied by either a negative or a positive ion, the resultant dipole field will be given by

$$E_{jz\bar{d}} = D_{jkz}(\mu_{kz})(\varepsilon/r^3), \quad (6a)$$

where j represents the ion occupying the centre of the cavity and k the ion the effect of which is to be calculated at the centre; \bar{d} indicates that the field is a dipole field.

For an incident field polarized in the X -direction, the corresponding expression is

$$E_{jx\bar{d}} = D_{jkx}(\mu_{kx})(\varepsilon/r^3), \quad (6b)$$

where D_{jkz} and D_{jkx} are the numerical values of the finite lattice sums in the deformed state. They may be evaluated using the expressions given in the appendix. In the stressed condition, the dipoles within the cavity produce a net field at the centre which in the undeformed state is zero, since $D_{jkz} = D_{jkx} = 0$.

In order to evaluate the Coulomb fields we again consider the effect of the incident field E_{iz} on the ions of the cavity. Under the influence of the field, the negative and positive charges of an ion will be displaced in opposite directions by the respective amounts s_1 and s_2 or s_k generally. If \tilde{e} is the effective charge (Fröhlich, 1949), and f_k is the oscillator strength of the ion, the dipole moment may be expressed as

$$f_k \tilde{e} s_k / \sqrt{4\pi} = (\mu_{kz}). \quad (7)$$

The displaced charges will create at the centre of the cavity a Coulomb field of net magnitude

$$E_{jzc} = (\beta \varepsilon / r^3) C_{jkz}(\alpha_k / f_k), \quad (8a)$$

where β denotes the number of valence electrons of the ion under consideration.

For a field polarized in the X -direction the corresponding expression is

$$E_{jxc} = (\beta \varepsilon / r^3) C_{jkx}(\alpha_k / f_k), \quad (8b)$$

where C_{jkz} and C_{jkx} are the numerical constants of the lattice. These may be evaluated using expressions given in the appendix.

When the cell is in the unstressed condition, the Coulomb field is zero, since $C_{jkz} = C_{jkx} = 0$.

Combining expressions (3), (6) and (8), we have

$$3(n_z^2 - 1) = N_j \alpha_j \left\{ (n_z^2 + 2) + (n^2 - 1) K_x \right\} + \left\{ D_{jkz} \frac{N_j \alpha_j \alpha_k}{r^3} + C_{jkz} \frac{N_j \alpha_j \alpha_k \beta}{f_k r^3} \right\} (n^2 + 2) \varepsilon \quad (9)$$

with a similar expression for n_x .

Here α_j is the polarizability of the ion under consideration and N_j , the number of such ions in unit volume.

4. Density and polarizability changes under stress

In addition to the anisotropy changes considered in the foregoing section, changes in density as well as the polarizability of the ions, occur under stress. To evaluate the density changes, consider a cube of unit dimensions subject to a stress in the Z -direction. If σ is the Poisson's ratio the strains ε and $\sigma\varepsilon$ produced parallel and perpendicular to the stress direction will alter the volume by an amount $\varepsilon(1 - 2\sigma)$. The change in the number of ions per unit volume is then $-\varepsilon(1 - 2\sigma)N_j$.

Polarizability changes under strain were first quantitatively considered by Mueller. He assumed the refractivities of the ions to be linear functions of the strain. In the presence of a combined field resulting from the continuum, the dipole and the Coulomb anisotropies, an effective polarizability of the ions may be assumed to arise in the following manner:

The dipole moment of the j th ion, in the presence of the resultant field is given by

$$\begin{aligned} (\mu_{jz})_{\text{dcp}} &= \alpha_j F_{jz} \text{ in the } Z\text{-direction} \\ (\mu_{jx})_{\text{dcp}} &= \alpha_j F_{jx} \text{ in the } X\text{-direction,} \end{aligned} \quad (10)$$

where

$$\begin{aligned} F_{jz} &= E_{iz} + E_{jzd} + E_{jzc} + K_z P_j \\ F_{jx} &= E_{ix} + E_{jxd} + E_{jxc} + K_x P_j. \end{aligned} \quad (11)$$

P_j in these expressions denotes the polarization of the medium per unit volume.

We may alternatively assume that the dipole moments of expressions (10) arise due to the effective polarizabilities α_{jz} or α_{jx} in the Z or X direction under an incident field E_{iz} or E_{ix} according to the equations

$$\begin{aligned} (\mu_{jz})_{\text{dcp}} &= \alpha_{jz} E_{iz} \\ (\mu_{jx})_{\text{dcp}} &= \alpha_{jx} E_{ix}. \end{aligned} \quad (12)$$

and

Equations (10), (11) and (12) together yield the following expressions:

$$\begin{aligned} \alpha_{jz} &= \alpha_j \left[1 + \left\{ \left(\frac{n^2 + 2}{3} \right) \left(D_{jkz} \frac{\alpha_k}{r^3} + C_{jkz} \frac{\beta \alpha_k}{r^3 f_k} \right) + \frac{K_z}{3} (n^2 - 1) \right\} \varepsilon \right] \\ \alpha_{jx} &= \alpha_j \left[1 + \left\{ \left(\frac{n^2 + 2}{3} \right) \left(D_{jkx} \frac{\alpha_k}{r^3} + C_{jkx} \frac{\beta \alpha_k}{r^3 f_k} \right) + \frac{K_x}{3} (n^2 - 1) \right\} \varepsilon \right] \end{aligned} \quad (13)$$

or

$$\begin{aligned} \alpha_{jz} &= \alpha_j (1 + \lambda_{kz} \varepsilon) \\ \alpha_{jx} &= \alpha_j (1 + \lambda_{kx} \varepsilon) \end{aligned}$$

in the form first given by Mueller who named λ_{kz} and λ_{kx} the strain polarizability constants. Here

$$\begin{aligned} \lambda_{kz} &= \left(\frac{n^2 + 2}{3} \right) \left(D_{jkz} \frac{\alpha_k}{r^3} + C_{jkz} \frac{\beta \alpha_k}{r^3 f_k} \right) + \frac{K_z}{3} (n^2 - 1) \\ \lambda_{kx} &= \left(\frac{n^2 + 2}{3} \right) \left(D_{jkx} \frac{\alpha_k}{r^3} + C_{jkx} \frac{\beta \alpha_k}{r^3 f_k} \right) + \frac{K_x}{3} (n^2 - 1). \end{aligned}$$

These expressions indicate that the polarizability constants are functions of wavelength and temperature, a conclusion in agreement with experimental facts.

5. Evaluation of the anisotropy constants

In evaluating the dipole and Coulomb fields, the following assumptions have been made:

(1) The field responsible for inducing the dipole and Coulomb effects is the effective field $E_{\text{eff.}} = E_i + P/3$, where E_i is the incident field and P is the polarization field.

(2) On deformation, the distance between any two atoms is changed in the same ratio as the corresponding bulk dimensions of the substance.

(3) On deformation, the unit cell within the cavity does not suffer a volume change.

Before deformation, the distance between any two atoms in the cell is r in the X , Y and Z directions. On the application of a stress T_z the distance in the three directions are altered to $z = r + \delta z$, $x = r - \delta x$, $y = r - \delta y$, where δx , δy and δz are the linear deformations caused by the stress. On the basis of assumptions 2 and 3 and neglecting the product and higher power terms in δx , δy and δz , the numerical constants $D_{jk(z \text{ or } x)}$ and $C_{jk(z \text{ or } x)}$ may be calculated. Their values are given in Table 1. They have been evaluated using expressions given in the appendix.

Table 1. Numerical constants

$D_{11z} = D_{22z} =$	0.2711	$D_{11x} = D_{22x} =$	-0.2711σ
$D_{12z} = D_{21z} =$	-1.1869	$D_{12x} = D_{21x} =$	1.1969σ
$C_{11z} = C_{22z} =$	1.6922	$C_{11x} = C_{22x} =$	-1.6922σ
$C_{12z} = C_{21z} =$	-4.2083	$C_{12x} = C_{21x} =$	4.2083σ

The numerical values of the finite lattice sums play an important role in determining the nature of the anisotropy and the polarizabilities of the ions in cubic crystals under consideration. It is found that these values depend very largely upon the nature of the assumptions made in calculating them. For example, if we assume with Banerjee & Mueller that the deformations in the perpendicular directions to stress are zero, it is found that the worked-out numerical constants agree well with the values given by them as shown in Tables 2(a) and (b). On the other hand, it is assumed that $\delta x = \delta y \neq 0$, the results are entirely different.

Table 2(a). Dipole anisotropy constants

Anisotropy constants	Authors		Banerjee $\delta x = \delta y = 0$
	$\delta x = \delta y \neq 0$	$\delta x = \delta y = 0$	
$B_{11z} = B_{22z}$	3.408	2.10	1.901
$B_{12z} = B_{21z}$	-14.92	-10.973	-9.9613
$B_{11x} = B_{22x}$	-3.408σ	-1.060	-0.9502
$B_{12x} = B_{21x}$	14.92σ	5.4865	4.9807

Where $B_{jk(z \text{ or } x)} = 4\pi D_{jk(z \text{ or } x)}$.

Table 2(b). Lorentz-Lorenz anisotropy constants

Anisotropy constants	Authors spherical cavity		Mueller (cubical cavity) $\delta x = \delta y = 0$
	$\delta x = \delta y \neq 0$	$\delta x = \delta y = 0$	
s_{11z}	0.2755	0.09	-0.06
s_{12z}	-2.107	-2.00	-1.91
s_{11x}	$0.1333 - 0.5422\sigma$	0.045	0.03
s_{12x}	$0.1333 + 2.374\sigma$	1.00	0.95

$$\text{Where } s_{jk(z \text{ or } x)} = \frac{2B_{jk(z \text{ or } x)}}{\pi N_k^3} + \frac{K_{(z \text{ or } x)}}{3}$$

$$N_k^3 = 4 \text{ for } k = 1 \text{ or } 2.$$

6. Change in refractive index under unidirectional stress

Equation (9) gives the refractive index of the crystal when the anisotropic fields alone are taken into consideration. Introducing the additional changes of polarizability and density of ions considered in Section 4, and assuming

$$\alpha = \alpha_1 + \alpha_2, \quad (14)$$

where α is the polarizability of the molecule, the final expression obtained for the change in the refractive index for light vibrations in the Z - and X -directions are given below:

$$\begin{aligned} dn_z = & -\frac{(n^2-1)(n^2+2)(1-2\sigma)\epsilon}{6n} - \frac{2(n^2-1)^2(n^2+5)}{45n} \\ & + \left\{ \frac{(n^2+2)^2(n^2+5)}{54n} [1.458 + 2.9005\beta(1/f_1 + 1/f_2)] \theta^2 \right. \\ & - \frac{(n^2-1)(n^2+2)(n^2+5)}{18n} \\ & \times \left[2.916 + \frac{4.2083\beta}{f_1} + \frac{7.5927\beta}{f_2} \right] \theta \\ & \left. + \frac{(n^2-1)^2(n^2+5)}{3n} \left[0.2711 + \frac{1.6922\beta}{f_2} \right] \right\} \epsilon \\ dn_x = & -\frac{(n^2-1)(n^2+2)(1-2\sigma)\epsilon}{6n} + \frac{(n^2-1)^2(n^2+5)}{45n} \\ & - \left\{ \frac{(n^2+2)^2(n^2+5)}{54n} [1.458 + 2.9005\beta(1/f_1 + 1/f_2)] \theta^2 \right. \\ & - \frac{(n^2-1)(n^2+2)(n^2+5)}{18n} \\ & \times \left[2.916 + \frac{4.2083\beta}{f_1} + \frac{7.5927\beta}{f_2} \right] \theta \\ & \left. + \frac{(n^2-1)^2(n^2+5)}{3n} \left[0.2711 + \frac{1.6922\beta}{f_2} \right] \right\} \sigma \epsilon, \end{aligned}$$

where

$$\theta = \frac{\alpha(1 \text{ or } 2)}{r^3}.$$

Putting

$$M = \frac{(n^2-1)^2(n^2+5)}{15n}, \quad L = \frac{(n^2-1)(n^2+2)}{6n}$$

and

$$A = \frac{(n^2+2)^2(n^2+5)}{54n} [1.458 + 2.9005\beta(1/f_1 + 1/f_2)]\theta^2$$

$$- \frac{(n^2-1)(n^2+2)(n^2+5)}{18n}$$

$$\times \left[2.916 + \frac{4.2083\beta}{f_1} + \frac{7.5927\beta}{f_2} \right] \theta$$

$$+ \frac{(n^2-1)^2(n^2+5)}{3n} \left[0.2711 + \frac{1.6922\beta}{f_2} \right]$$

the strain-optical coefficients as defined in equations (1) can be conveniently expressed in the following form:

$$P_{11} - P_{12} = (2/n^3)\{3M - (1 + \sigma)A\}$$

$$P_{11} + 2P_{12} = (2/n^3)(3L - A)(1 - 2\sigma) \quad (15)$$

and

$$(n^2/6)(P_{11} + 2P_{12}) = L(1 - \lambda_0),$$

where

$$\lambda_0 = 2\sigma + \frac{A(1 - 2\sigma)}{3L}.$$

APPENDIX

$$(D_{11z} = D_{22z})(4\pi\epsilon/r^3)$$

$$= 3z^2\{(z^2 + x^2)^{-5/2} + (y^2 + z^2)^{-5/2}\}$$

$$- \{(x^2 + y^2)^{-3/2} + (y^2 + z^2)^{-3/2} + (z^2 + x^2)^{-3/2}\}.$$

$$(D_{12z} = D_{21z})(4\pi\epsilon/r^3)$$

$$= 12z^2R^{-5} + 3z^{-3} - \{4R^{-3} + x^{-3} + y^{-3} + z^{-3}\}.$$

$$(D_{11x} = D_{22x})(4\pi\epsilon/r^3)$$

$$= 3x^2\{(x^2 + y^2)^{-5/2} + (x^2 + z^2)^{-5/2}\}$$

$$- \{(x^2 + y^2)^{-3/2} + (y^2 + z^2)^{-3/2} + (z^2 + x^2)^{-3/2}\}.$$

$$(D_{12x} = D_{21x})(4\pi\epsilon/r^3)$$

$$= 12x^2R^{-5} + 3x^{-3} - \{4R^{-3} + x^{-3} + y^{-3} + z^{-3}\}.$$

$$C_{j kz} \frac{\alpha_k E_{\text{eff.}} \epsilon / (4\pi)}{f_k \epsilon r^3}$$

$$= (z - s_k)^{-2} + 4(z - s_k)\{x^2 + y^2 + (z - s_k)^2\}^{-3/2}$$

$$- [(z + s_k)^{-2} + 2s_k(x^2 + s_k^2)^{-3/2} + 2s_k(y^2 + s_k^2)^{-3/2}$$

$$+ 4(z + s_k)\{x^2 + y^2 + (z + s_k)^2\}^{-3/2}]$$

where $j = 1$, and $k = 2$ or $j = 2$ and $k = 1$.

$$C_{j kz} \frac{\alpha_k E_{\text{eff.}} \epsilon / (4\pi)}{f_k \epsilon r^3}$$

$$= 2(z - s_k)\{x^2 + (z - s_k)^2\}^{-3/2}$$

$$+ 2(z - s_k)\{y^2 + (z - s_k)^2\}^{-3/2}$$

$$- 4s_k\{(x^2 + y^2 + s_k^2)\}^{-3/2}$$

$$- 2(z + s_k)\{x^2 + (z + s_k)^2\}^{-3/2}$$

$$- 2(z + s_k)\{y^2 + (z + s_k)^2\}^{-3/2}$$

where $j = k = 1$ or $j = k = 2$.

$$C_{j kx} \frac{\alpha_k E_{\text{eff.}} \epsilon / (4\pi)}{f_k \epsilon r^3}$$

$$= 2(x - s_k)\{y^2 + (x - s_k)^2\}^{-3/2}$$

$$+ 2(x - s_k)\{z^2 + (x - s_k)^2\}^{-3/2}$$

$$- 4s_k\{(y^2 + z^2 + s_k^2)\}^{-3/2} - 2(x + s_k)\{y^2 + (x + s_k)^2\}^{-3/2}$$

$$- 2(x + s_k)\{z^2 + (x + s_k)^2\}^{-3/2}$$

where $j = k = 1$ or $j = k = 2$.

$$C_{j kx} \frac{\alpha_k E_{\text{eff.}} \epsilon / (4\pi)}{f_k \epsilon r^3}$$

$$= (x - s_k)^{-2} + 4(x - s_k)\{y^2 + z^2 + (x - s_k)^2\}^{-3/2}$$

$$- (x + s_k)^{-2} + 2s_k(y^2 + s_k^2)^{-3/2} + 2s_k(z^2 + s_k^2)^{-3/2}$$

$$+ 4(x + s_k)\{y^2 + z^2 + (x + s_k)^2\}^{-3/2}$$

where $j = 1$ and $k = 2$ or $j = 2$ and $k = 1$.

References

- BANERJEE, K. (1927). *Indian J. Phys.* **2**, 195.
 BRAGG, W. L. (1924a). *Proc. Roy. Soc. A*, **105**, 370.
 BRAGG, W. L. (1924b). *Proc. Roy. Soc. A*, **106**, 346.
 BRAYBORN, J. E. H. (1953). *Proc. Phys. Soc. B*, **66**, 617.
 BURSTEIN, E. & SMITH, P. L. (1949). *Proc. Indian Acad. Sci.* **28**, 377.
 FRÖHLICH, H. (1949). *Theory of Dielectrics*. Oxford: Clarendon Press.
 HAVELOCK, T. H. (1908). *Proc. Roy. Soc. A*, **80**, 31.
 HERZFELD, K. F. (1928). *J. Opt. Soc. Amer.* **17**, 26.
 HERZFELD, K. F. & LEE, R. H. (1933). *Phys. Rev.* **44**, 625.
 MUELLER, H. (1935a). *Phys. Rev.* **47**, 947.
 MUELLER, H. (1935b). *Physics*, **6**, 179.
 POCKELS, F. (1906). *Lehrbuch der Kristalloptik*. Berlin: Teubner.
 POINDESTER, E. (1955). *Amer. Min.* **40**, 1032.